

3,3,4,4,5,5,6,6,7,7,8,8,8-Tridecafluorooctan-1-ol
647-42-7 | DTXSID5044572

Model Performance

Model	Data
-------	------

Weighted KNN model					
5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 4.47 days

Global applicability domain: Outside

Local applicability domain index: 2.75e-01

Confidence level: 7.64e-01

Nearest Neighbors from the Training Set

Image not found

Tetradeca-1,13-diene

Measured: 367

Predicted: 8.69

Image not found

2-Methylheptane

Measured: 12.5

Predicted: 3.99

Image not found

2-Methylhexane

Measured: 12.5

Predicted: 5.54

Image not found

2-Methyloctane

Measured: 40.7

Predicted: 4.23